

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120715\
 Data File : BF083568.D
 Acq On : 7 Dec 2015 20:58
 Operator : UM/IZ
 Sample : G4579-05
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP3(6-12)

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-BF120415.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	3.550	161	163	177	rBV	770677	1675032	34.21%	3.654%
2	3.996	200	202	221	rBV	3187889	4402841	89.93%	9.605%
3	5.287	312	315	324	rBV	3367638	4895879	100.00%	10.680%
4	5.413	324	326	329	rVV	3552788	4468243	91.27%	9.747%
5	5.721	350	353	359	rBV	806410	1028450	21.01%	2.244%
6	5.939	369	372	381	rVB	2739379	3483019	71.14%	7.598%
7	6.133	384	389	393	rVB2	82516	155822	3.18%	0.340%
8	6.202	393	395	397	rBV	29307	49075	1.00%	0.107%
9	6.544	422	425	428	rBV	1795058	2773157	56.64%	6.050%
10	6.830	447	450	452	rBV2	53344	100010	2.04%	0.218%
11	7.253	480	487	489	rBV5	22773	58457	1.19%	0.128%
12	7.390	495	499	505	rBV4	21780	52774	1.08%	0.115%
13	7.619	516	519	525	rBV	960885	1376562	28.12%	3.003%
14	7.962	546	549	552	rBV3	31504	55954	1.14%	0.122%
15	9.173	652	655	660	rBV2	28974	53575	1.09%	0.117%
16	9.368	668	672	675	rBV	3589369	4711655	96.24%	10.278%
17	10.053	729	732	735	rBV	896013	1079212	22.04%	2.354%
18	10.408	760	763	769	rBV2	1070666	1602157	32.72%	3.495%
19	10.819	792	799	801	rBV2	22456	55031	1.12%	0.120%
20	11.185	827	831	834	rBV2	25976	52602	1.07%	0.115%
21	11.253	834	837	840	rVV	180256	232081	4.74%	0.506%
22	11.619	864	869	871	rBV	51190	121282	2.48%	0.265%
23	11.699	873	876	879	rBV	1949741	2638220	53.89%	5.755%
24	12.031	898	905	909	rBV	159924	372112	7.60%	0.812%
25	12.088	909	910	913	rVV2	51204	97197	1.99%	0.212%
26	12.145	913	915	917	rVV2	52185	93405	1.91%	0.204%
27	12.225	920	922	925	rVB2	28223	52699	1.08%	0.115%
28	12.442	939	941	944	rBV	51364	96213	1.97%	0.210%
29	12.762	966	969	971	rBV	89068	131198	2.68%	0.286%
30	12.808	971	973	979	rVB	973753	1324053	27.04%	2.888%
31	13.459	1027	1030	1033	rBV	33341	51700	1.06%	0.113%
32	13.722	1051	1053	1057	rBV3	28621	65708	1.34%	0.143%
33	13.859	1062	1065	1073	rBV	267310	449027	9.17%	0.980%
34	14.237	1095	1098	1103	rVB2	37371	88484	1.81%	0.193%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.579	1125	1128	1132	rBV	73088	122079	2.49%	0.266%
36	15.140	1174	1177	1181	rBV2	143143	247021	5.05%	0.539%
37	15.265	1185	1188	1191	rVV	57717	84146	1.72%	0.184%
38	15.437	1200	1203	1206	rBV	2365262	3398688	69.42%	7.414%
39	16.317	1276	1280	1289	rBV	458433	628486	12.84%	1.371%
40	16.443	1289	1291	1294	rBV	33963	60838	1.24%	0.133%
41	16.934	1332	1334	1339	rBV	216216	374013	7.64%	0.816%
42	17.014	1339	1341	1347	rVB	693568	1002430	20.47%	2.187%
43	17.757	1404	1406	1410	rBV	168609	236564	4.83%	0.516%
44	18.066	1430	1433	1435	rBV	89772	108201	2.21%	0.236%
45	18.168	1439	1442	1444	rBV	212481	230856	4.72%	0.504%
46	18.443	1462	1466	1469	rBV2	86134	196130	4.01%	0.428%
47	18.648	1482	1484	1490	rBV	681046	898017	18.34%	1.959%
48	19.106	1521	1524	1525	rBV2	38893	61715	1.26%	0.135%
49	19.734	1577	1579	1582	rVB4	25785	50501	1.03%	0.110%
50	20.306	1627	1629	1636	rVB7	23576	60041	1.23%	0.131%
51	21.883	1763	1767	1772	rBV6	42398	138074	2.82%	0.301%

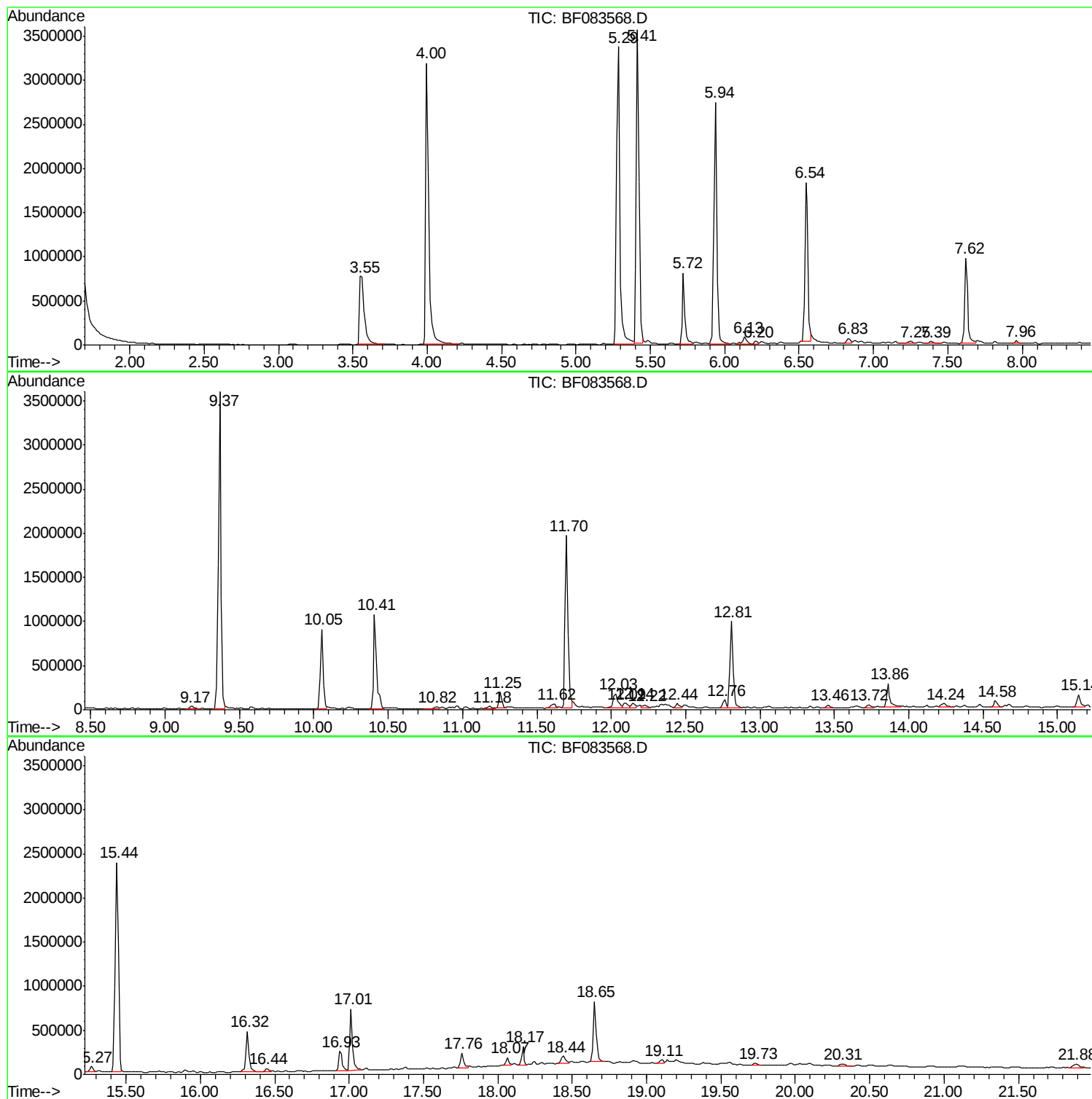
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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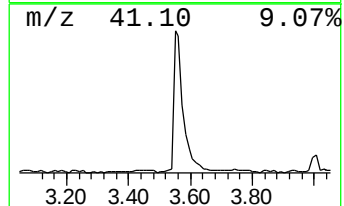
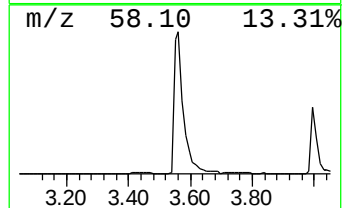
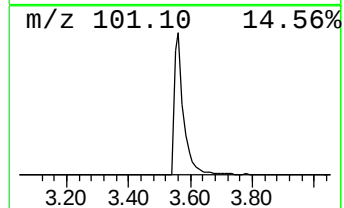
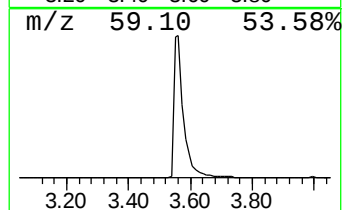
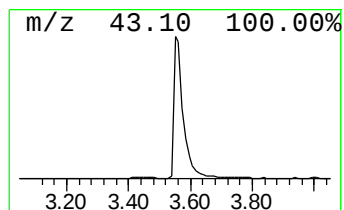
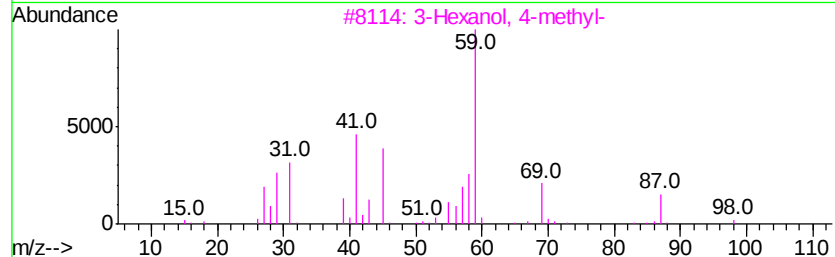
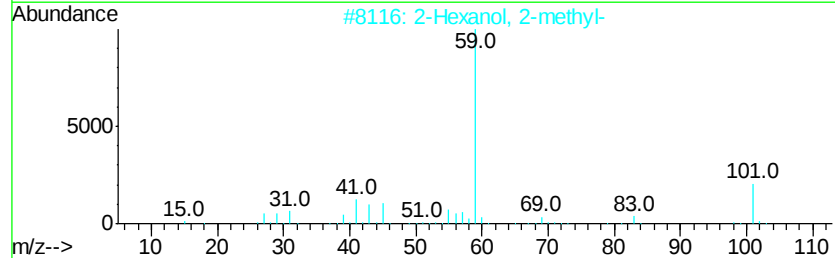
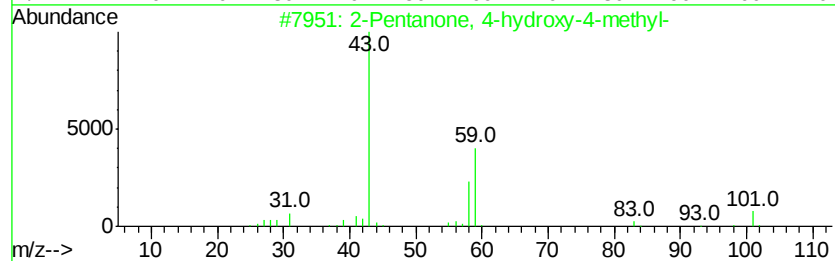
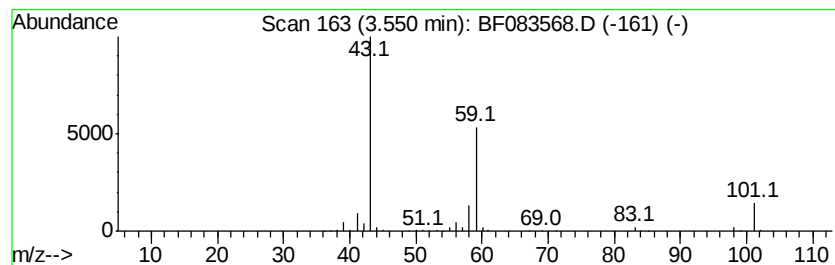
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
3.55	32.57 ng	1675030	1,4-Dichlorobenzene-d4	5.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
5		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9



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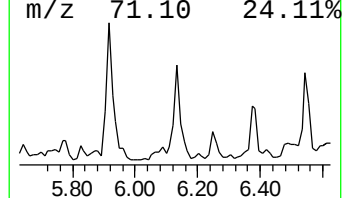
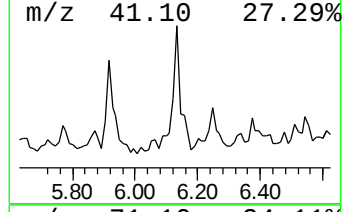
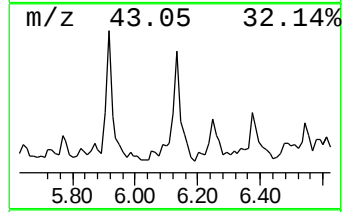
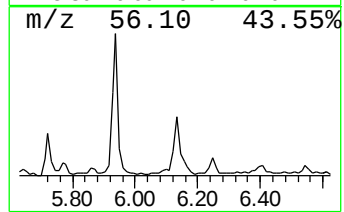
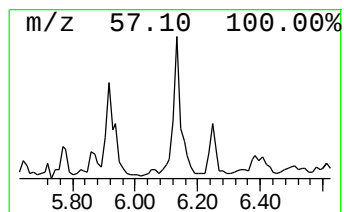
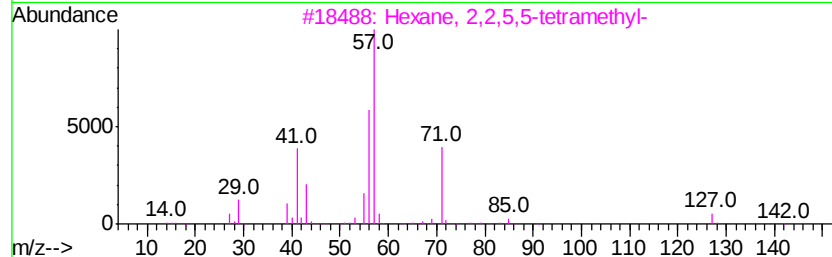
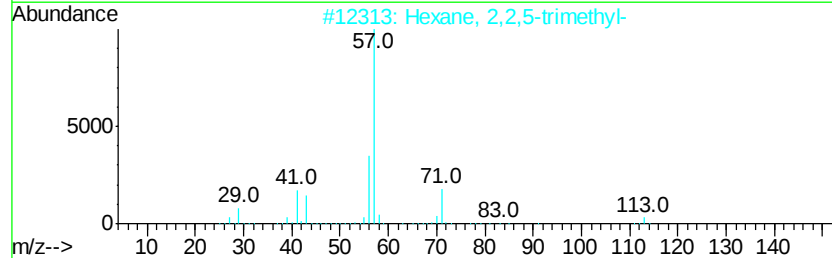
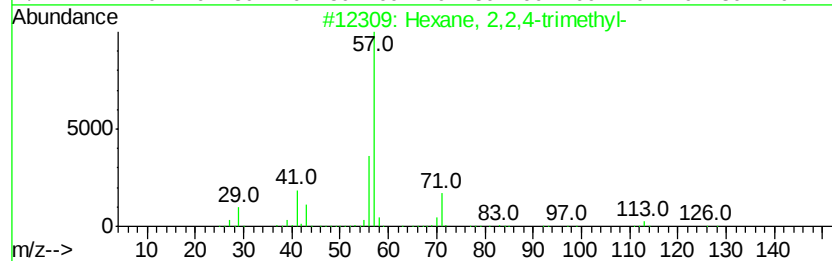
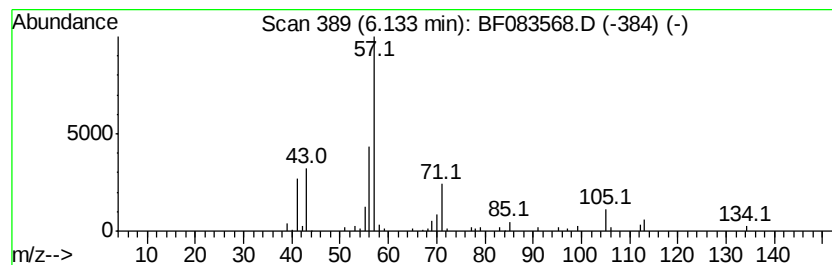
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexane, 2,2,4-trimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.13	3.03 ng	155822	1,4-Dichlorobenzene-d4	5.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
2		Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	59
3		Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	50
4		Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	47
5		Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	47



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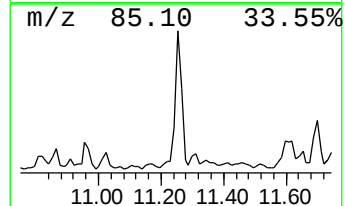
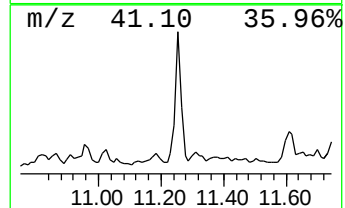
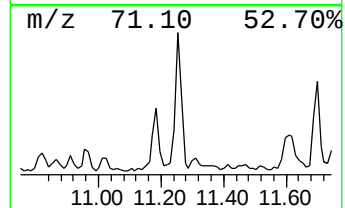
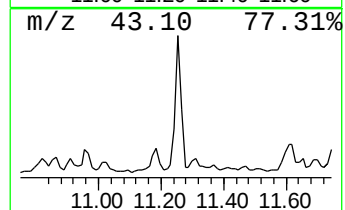
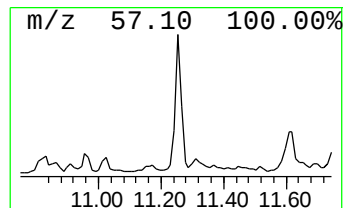
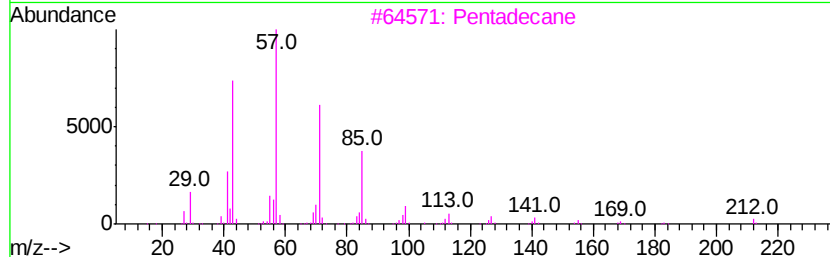
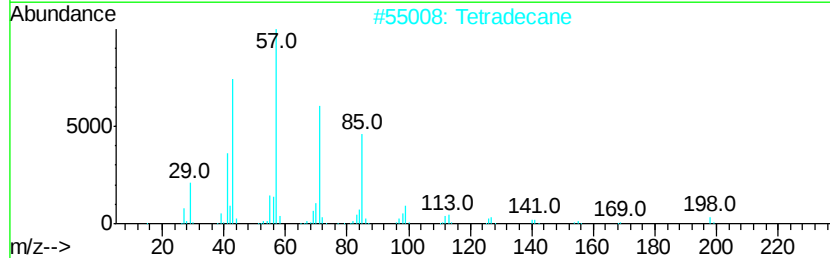
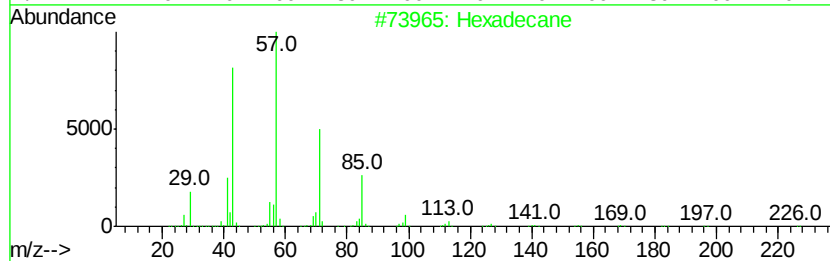
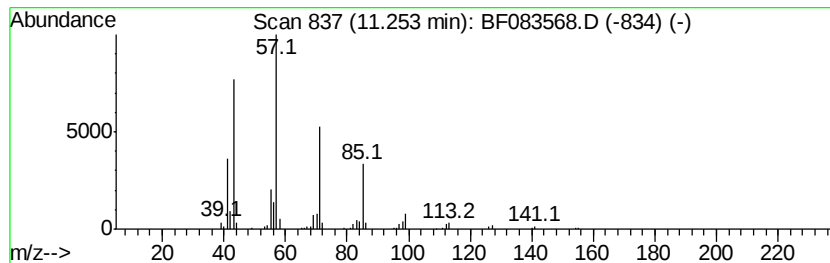
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.25	2.90 ng	232081	Acenaphthene-d10	10.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	91
2	Tetradecane		198	C14H30	000629-59-4	90
3	Pentadecane		212	C15H32	000629-62-9	86
4	Decane, 3-bromo-		220	C10H21Br	030571-71-2	64
5	Heptadecane, 2,6,10,14-tetramethyl-		296	C21H44	018344-37-1	59



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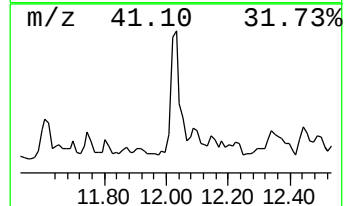
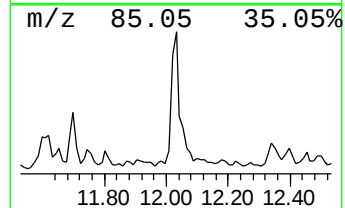
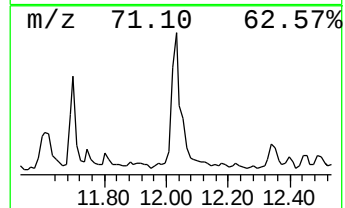
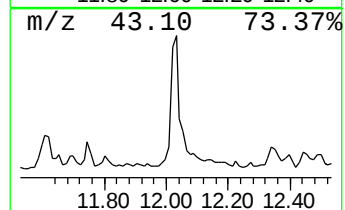
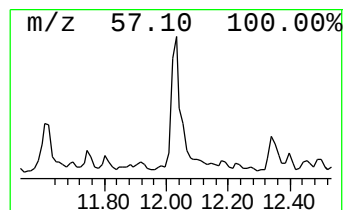
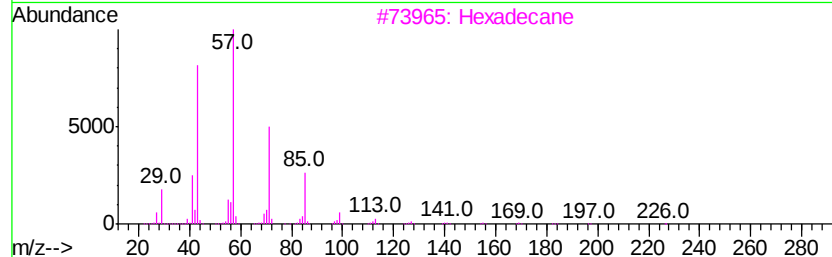
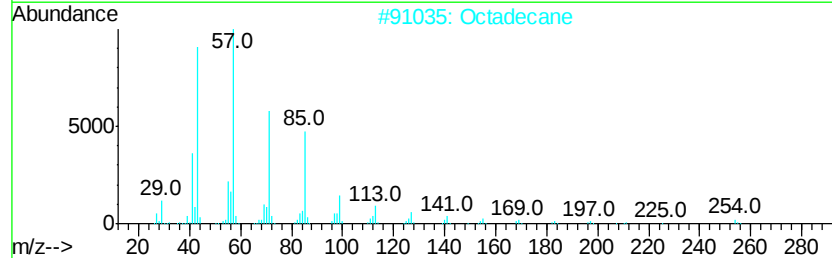
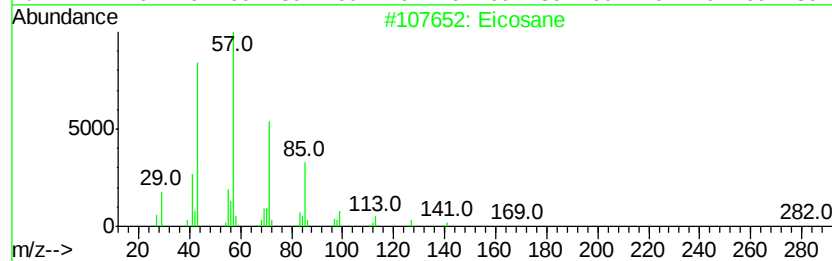
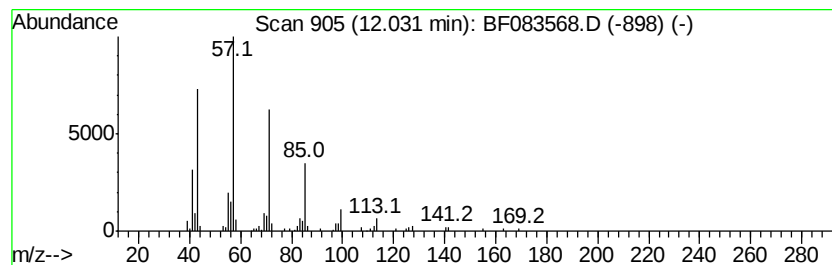
Instrument :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.03	5.62 ng	372112	Phenanthrene-d10		12.81
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Octadecane	254	C18H38	000593-45-3	90
3	Hexadecane	226	C16H34	000544-76-3	86
4	Heptacosane	380	C27H56	000593-49-7	83
5	Tetracosane	338	C24H50	000646-31-1	78



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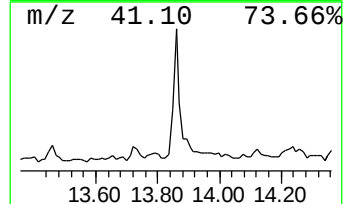
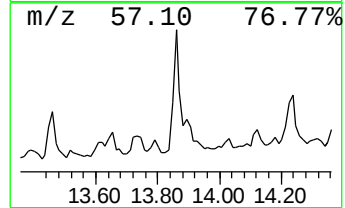
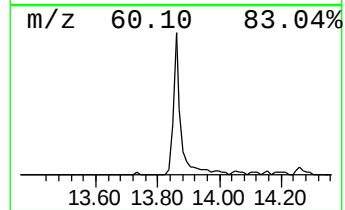
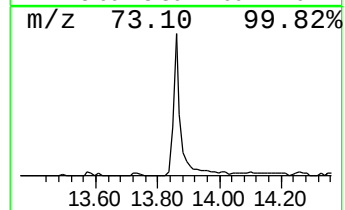
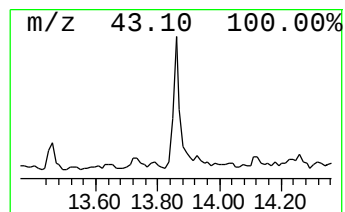
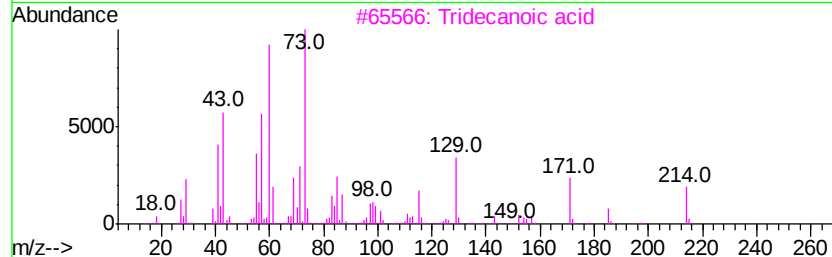
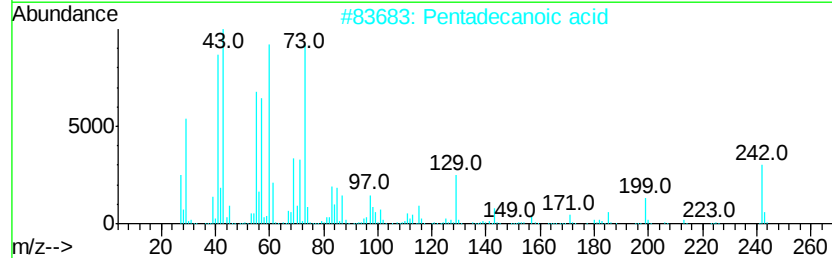
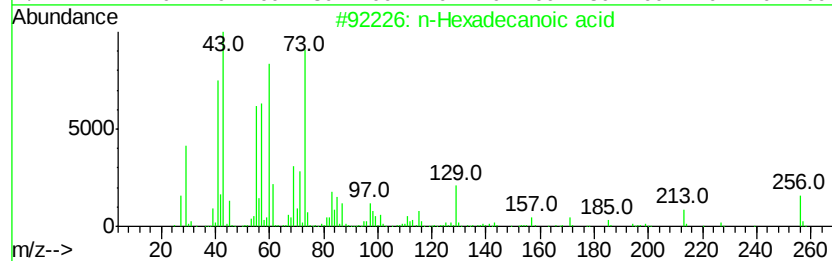
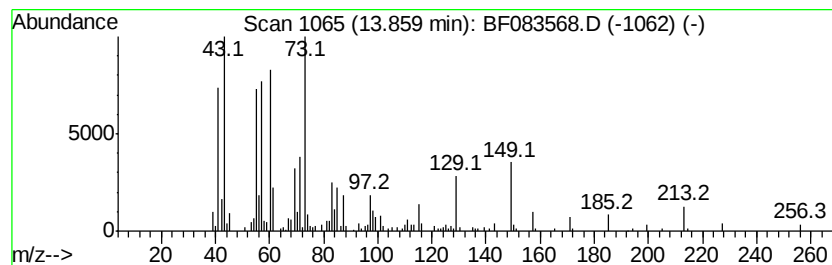
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ClientSampleId :
TP3(6-12)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.86	6.78 ng	449027	Phenanthrene-d10	12.81	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF120715\
Data File : BF083568.D
Acq On : 7 Dec 2015 20:58
Operator : UM/IZ
Sample : G4579-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

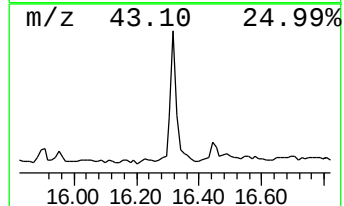
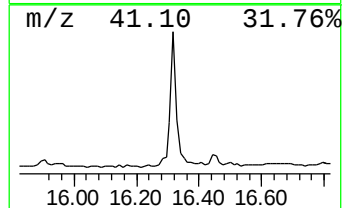
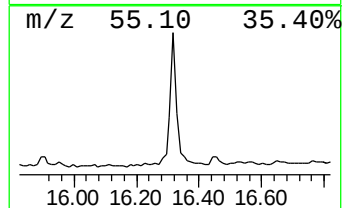
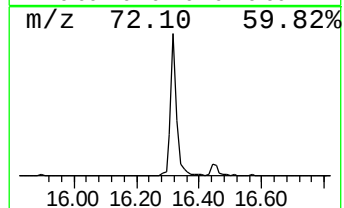
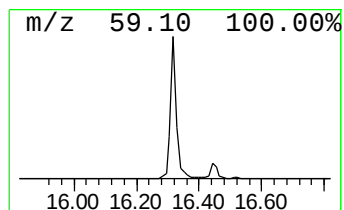
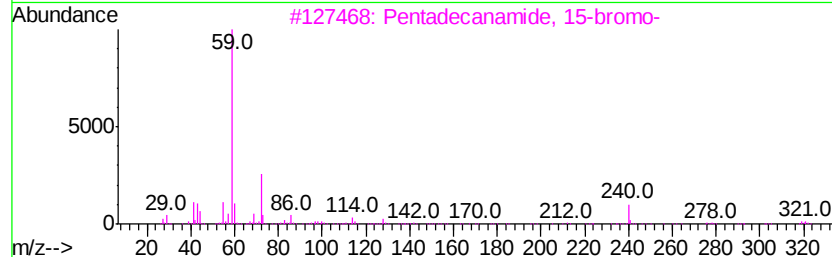
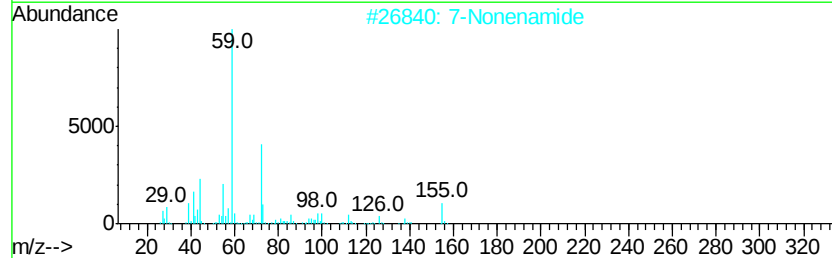
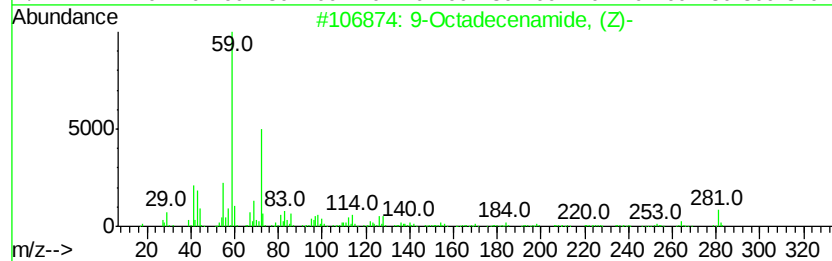
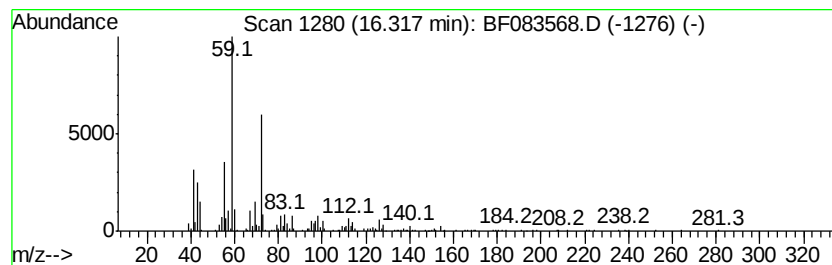
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.32	12.54 ng	628486	Chrysene-d12	17.01
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	9-Octadecenamide, (Z)-	281 C18H35NO	000301-02-0	78
2	7-Nonenamide	155 C9H17NO	090949-53-4	64
3	Pentadecanamide, 15-bromo-	319 C15H30BrNO	1000163-86-1	59
4	Hexadecanamide	255 C16H33NO	000629-54-9	56
5	Tetradecanamide	227 C14H29NO	000638-58-4	56



Data Path : Z:\HPCHEM1\BNA F\DATA\BF120715\
Data File : BF083568.D
Acq On : 7 Dec 2015 20:58
Operator : UM/IZ
Sample : G4579-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

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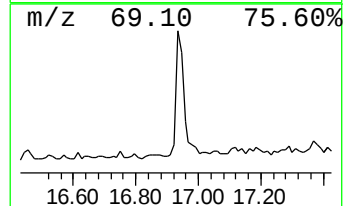
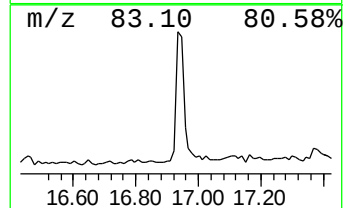
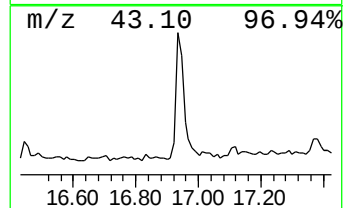
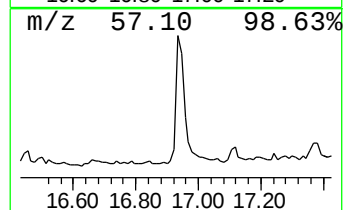
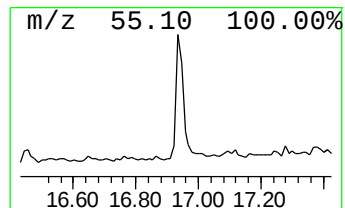
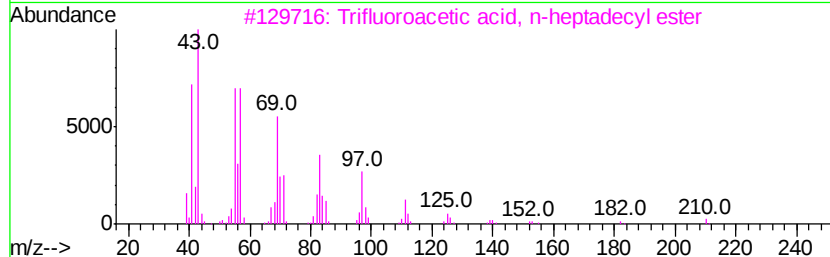
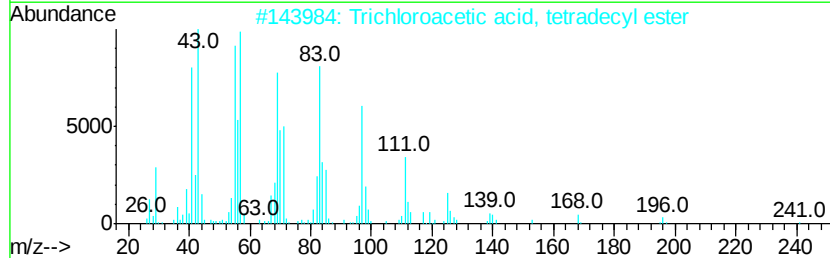
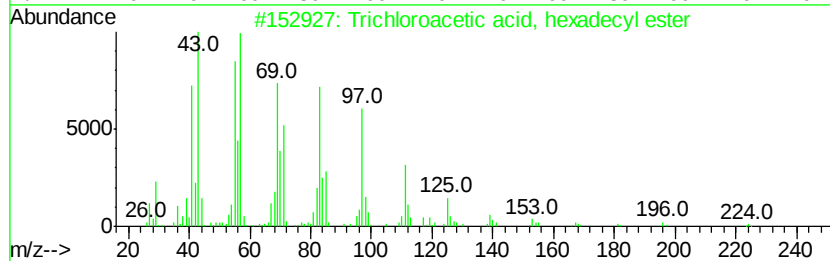
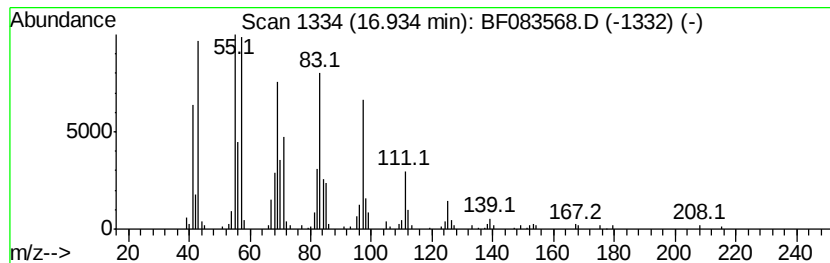
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.93	7.46 ng	374013	Chrysene-d12	17.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	94
3		Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91
4		11-Tricosene	322	C23H46	052078-56-5	91
5		1-Nonadecene	266	C19H38	018435-45-5	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120715\
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Acq On : 7 Dec 2015 20:58
Operator : UM/IZ
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Misc :
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Instrument :
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ClientSampleId :
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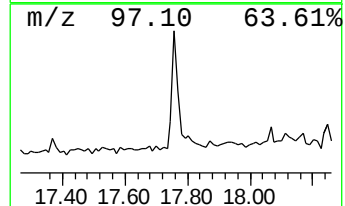
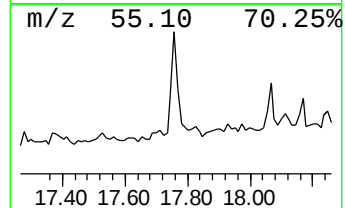
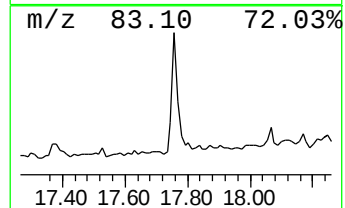
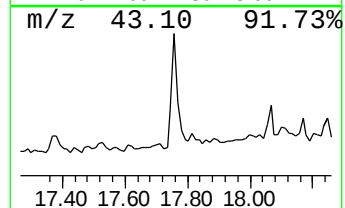
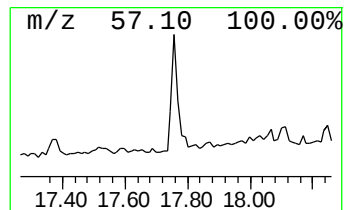
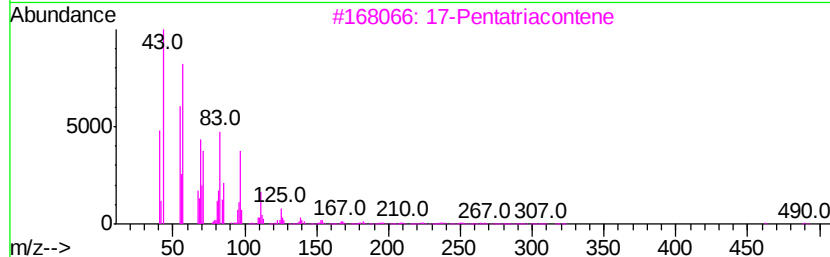
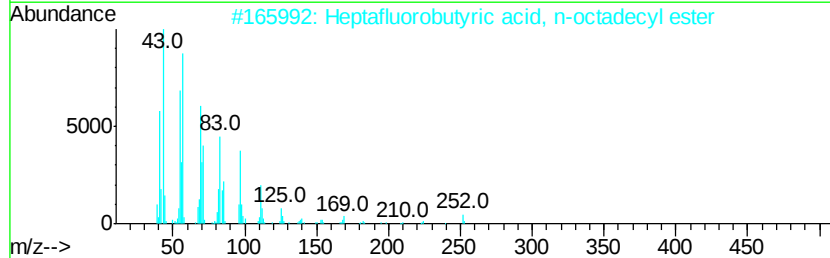
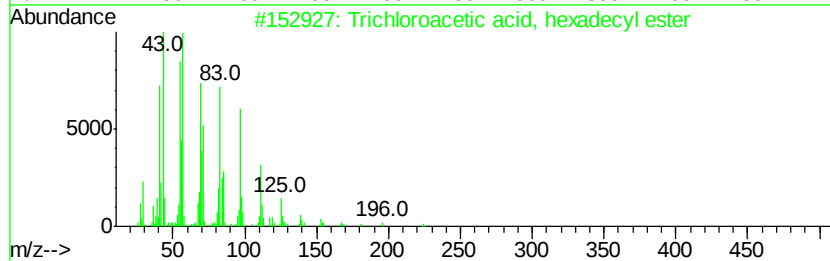
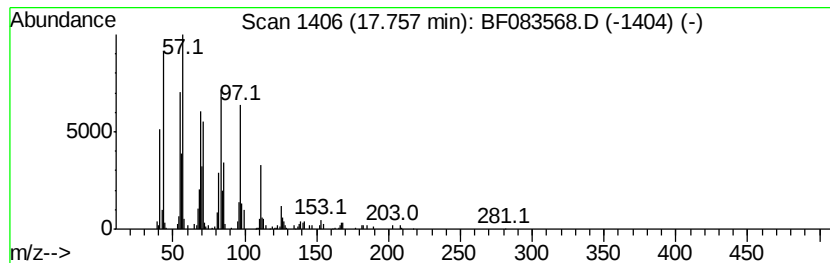
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Heptafluorobutyric acid, n-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.76	4.72 ng	236564	Chrysene-d12	17.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3		17-Pentatriacontene	491	C35H70	006971-40-0	91
4		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
5		1-Docosene	308	C22H44	001599-67-3	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120715\
Data File : BF083568.D
Acq On : 7 Dec 2015 20:58
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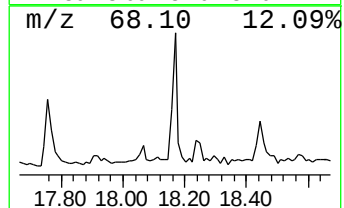
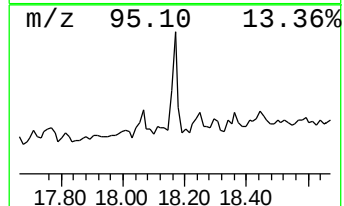
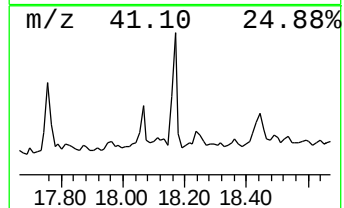
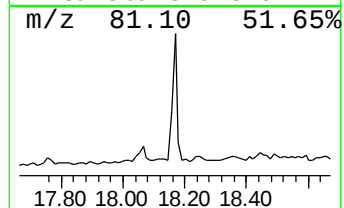
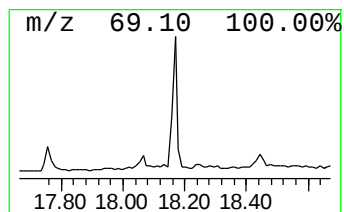
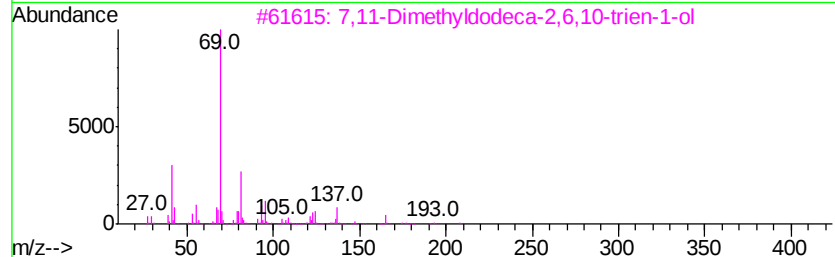
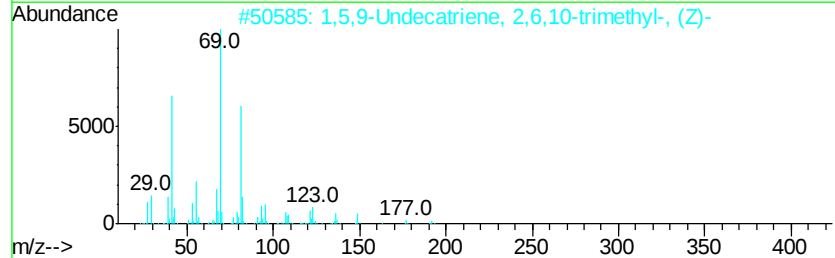
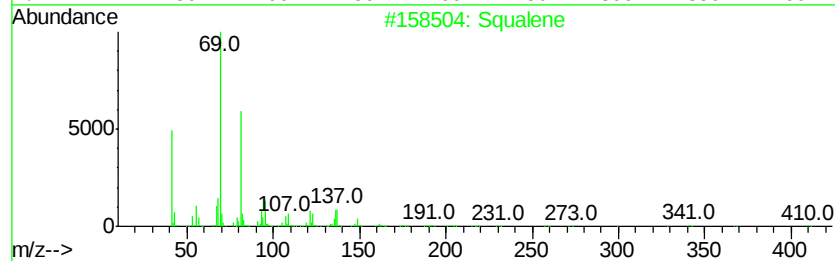
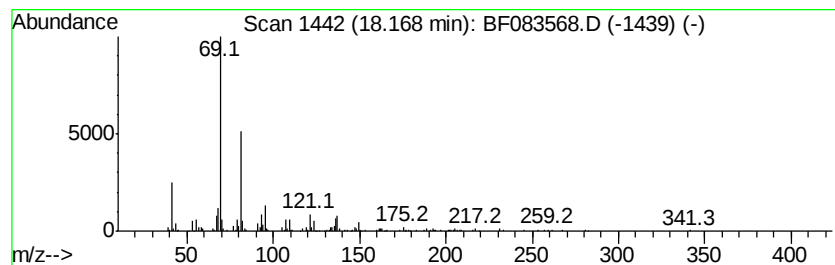
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.17	5.14 ng	230856	Perylene-d12	18.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	90
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	90
4		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
5		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120715\
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Acq On : 7 Dec 2015 20:58
Operator : UM/IZ
Sample : G4579-05
Misc :
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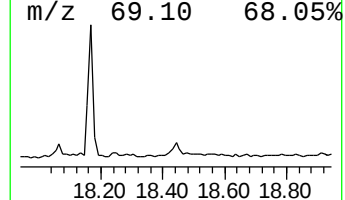
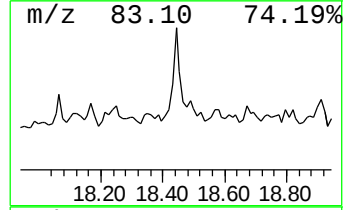
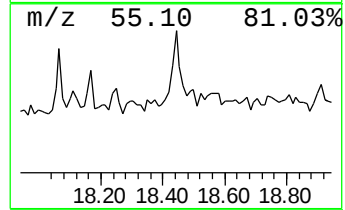
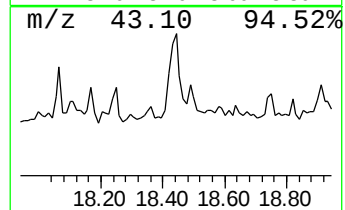
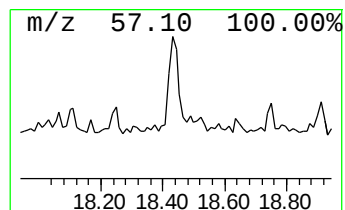
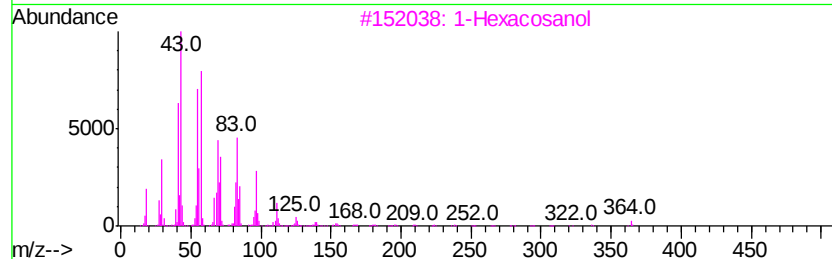
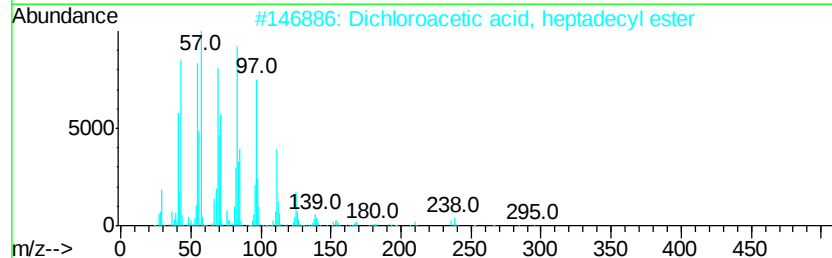
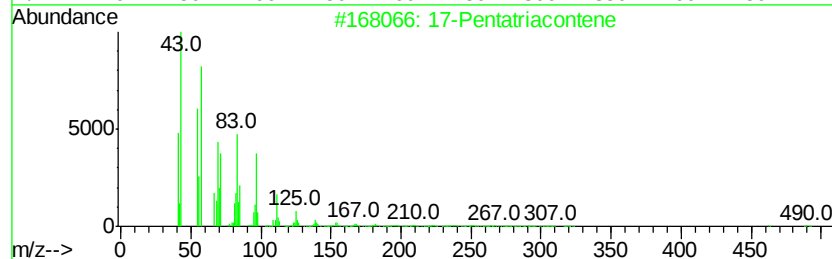
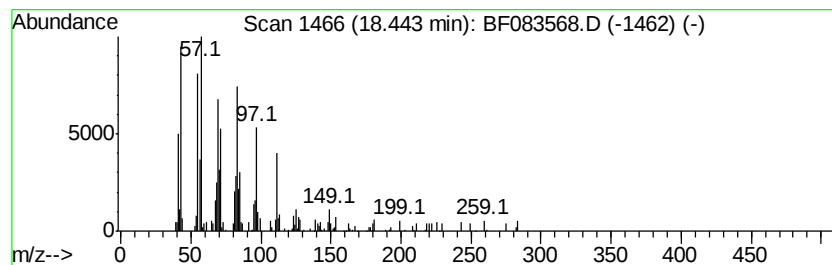
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 17-Pentatriacontene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.44	4.37 ng	196130	Perylene-d12	18.65
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	17-Pentatriacontene	491 C35H70	006971-40-0	87
2	Dichloroacetic acid, heptadecyl ...	366 C19H36Cl2O2	1000282-98-2	83
3	1-Hexacosanol	382 C26H54O	000506-52-5	81
4	1-Tetracosanol	354 C24H50O	000506-51-4	81
5	Trichloroacetic acid, tetradecyl...	358 C16H29Cl3O2	074339-52-9	80



Data Path : Z:\HPCHEM1\BNA F\DATA\BF120715\
Data File : BF083568.D
Acq On : 7 Dec 2015 20:58
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TP3(6-12)

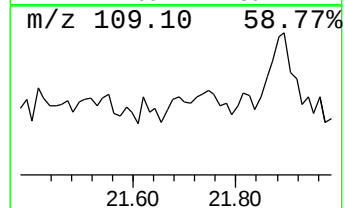
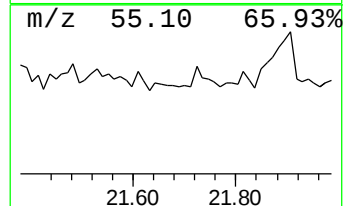
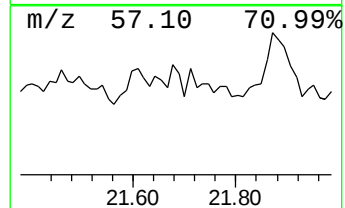
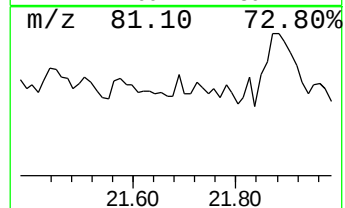
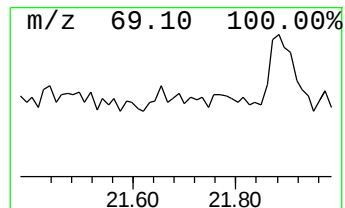
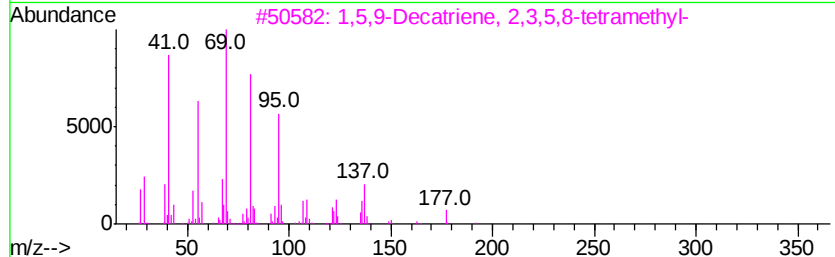
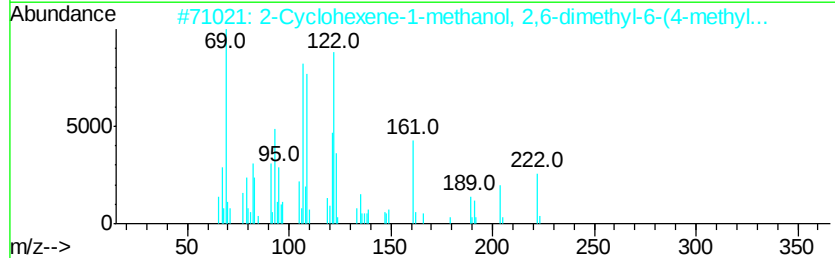
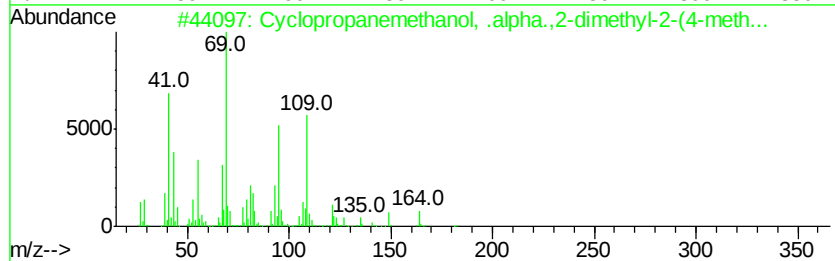
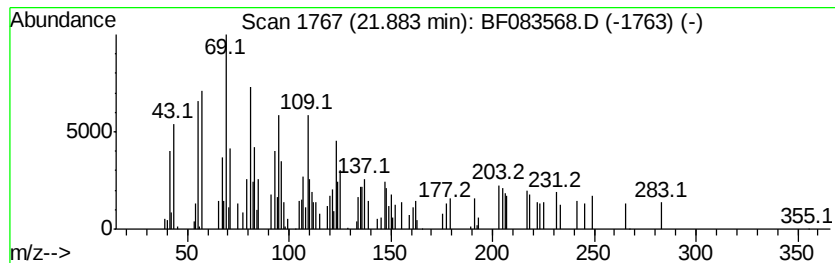
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 unknown21.88 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.88	3.08 ng	138074	Perylene-d12	18.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopropanemethanol, .alpha.,2-...	182	C12H22O	121959-70-4	47
2		2-Cyclohexene-1-methanol, 2,6-di...	222	C15H26O	038142-34-6	46
3		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	43
4		Sesquirosefuran	218	C15H22O	039007-93-7	43
5		Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	000547-60-4	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120715\
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Acq On : 7 Dec 2015 20:58
Operator : UM/IZ
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP3(6-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	3.55	32.6	ng	1675030	1	5.72	1028450	20.0
Hexane, 2,2,4-tri...	6.13	3.0	ng	155822	1	5.72	1028450	20.0
Hexadecane	11.25	2.9	ng	232081	3	10.41	1602160	20.0
Eicosane	12.03	5.6	ng	372112	4	12.81	1324050	20.0
n-Hexadecanoic acid	13.86	6.8	ng	449027	4	12.81	1324050	20.0
9-Octadecenamide,...	16.32	12.5	ng	628486	5	17.01	1002430	20.0
Trichloroacetic a...	16.93	7.5	ng	374013	5	17.01	1002430	20.0
Heptafluorobutyri...	17.76	4.7	ng	236564	5	17.01	1002430	20.0
Squalene	18.17	5.1	ng	230856	6	18.65	898017	20.0
17-Pentatriacontene	18.44	4.4	ng	196130	6	18.65	898017	20.0
unknown21.88	21.88	3.1	ng	138074	6	18.65	898017	20.0